

Many body effects on *c*- axis properties: out of plane coherence and bilayer splitting.

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The out-of-plane hopping in layered metals with strong electronic correlation is analyzed theoretically. By studying the effects of in-plane interactions on the interlayer tunnelling we investigate one of the oldest unresolved problems of high- T_c cuprates, the so-called bilayer splitting.

The strong electron-electron interactions within each layer reduce the quasiparticle weight, and modify the hopping between layers. We analyze the effect of the in-plane correlations on the interlayer hopping using a Renormalization Group scheme already applied to the problem of interlayer coherence. The bilayer band splitting acquires a significant temperature and doping dependence, and can be completely suppressed when the Fermi energy coincides with a Van Hove singularity.

I. INTRODUCTION

The strong anisotropy and anomalous *c*- axis properties of the high-temperature cuprate superconductors are among the most relevant features of these layered materials and have greatly conditioned the theoretical scenario¹. Although intensively investigated, the out-of-plane behaviour of the cuprates is not yet well understood. The role of the multiple layers and its relevance in the critical temperature T_c and optimal doping values of different compounds, is not settled yet².

One of the most interesting issues has been the interaction between CuO_2 planes in materials with two planes per unit cell. As predicted by early band structure calculations, the interaction between planes would split their electronic structure in bonding and antibonding bands, the so-called bilayer band splitting. This splitting was expected to be maximum at $(\pi, 0)$ and vanish along $(0, 0) - (\pi, \pi)$, by symmetry effects³. The absence of the BS on early angle-resolved photoemission experiments on $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) aroused great expectation⁴, in connection with the interlayer pair tunneling model¹. Recently, angle-resolved photoemission spectroscopy (ARPES) data on bilayer cuprate Bi2212 have reported a bilayer band splitting (BS) between bonding and antibonding bands in the Brillouin zone (BZ) antinodal region of overdoped samples, above and below T_c ^{5,6}. The bilayer energy splitting, due to the intrabilayer coupling, is of about 100 meV in the $(\pi, 0)$ region in the normal state and of about 20 meV in the superconducting state. The momentum and energy behavior of the BS agree qualitatively with the bilayer Hubbard model calculations⁷. The report of BS as well in underdoped and optimally doped Bi2212 samples, not resolved before, by ARPES measurements with different photon energies and high momentum and energy resolution⁸, should be seriously considered and put constraints in existing theories and data analysis^{9,10,11}. The existence of BS in all doping ranges seems to confront with the coherence issue. In this context, a crossover in the phase diagram between the low temperature, overdoped side

with coherent electronic excitations, and the high temperature, underdoped side where this coherence is lost, has been reported from ARPES data and resistivity measurements of Bi2212¹², in good agreement with theoretical predictions¹³, and with optical conductivity results¹⁴ from which the coherent-to-incoherent crossover as a function of doping has been reported. In the overdoped region, conventional Fermi liquid behavior is expected while in the underdoped region correlation effects would deviate from the conventional physics yielding exotic behavior, in agreement with the most common doping-temperature phase diagram for the cuprates. A crossover from insulating-like, at high temperatures, to metallic-like character at low temperatures in the direction perpendicular to the layers, while being metallic within the layers, has been recently reported by Valla *et al* from ARPES measurements in layered, non-superconducting materials¹⁵, the change of effective dimensionality being correlated with the existence or non-existence of coherence within the layers. The splitting of the CuO_2 -plane states in the whole doping range would imply the coherence of electronic states in the *c* axis at least to the intracell distance between the two planes. At present, consensus on the existence of BS has been reached only in the overdoped regime, while in optimally doped and underdoped regime there is not a clear agreement. Recently¹⁶ high-resolution ARPES experiments on Bi2212 covering the entire doping range, and with photons of 22 eV and 47 eV (ARPES matrix element effects for photons of 47 eV strongly enhance the antibonding component of the bilayer in the $(\pi, 0)$ region of the BZ) suggest that the size of the intracell coupling is only weakly dependent on the doping level, therefore some coherent coupling exists between the CuO_2 planes of the unit cell even in underdoped system. To explain the *c*-axis transport measurements where an insulating ρ_c behavior is reported in underdoped samples, ref¹⁶ argue that intracell perpendicular hopping will dominate the BS while the intercell perpendicular hopping will control the *c*-axis resistivity ρ_c .

It is the purpose of this paper to analyze the role played

by many-body effects on the interlayer coupling of high- T_c superconductors and its effects on the bilayer splitting.

II. MODEL AND METHOD

In spite of the great theoretical effort in high- T_c superconductivity, there is not yet a theory of consensus. The Hubbard hamiltonian is among the most studied models in the hight- T_c superconductors field, since it explains the main low-energy physics results of the CuO_2 planes, which are the common blocks to all families and where it is assumed to lie the main physics of the cuprates. The insulating parent compound is obtained at half-filling with antiferromagnetic correlations, while upon doping the known phase diagram is obtained. The stripe phase as well as d-wave superconductivity are well described within the Hubbard model¹⁷. Furthermore, in the overdoped regime, where Fermi-liquid-like behavior seems to hold, ARPES data of Bi2212 qualitatively agree with bilayer Hubbard model calculation results for the energy splitting⁵, a experimental intrabilayer hopping $t_{\perp,exp} \approx 44$ meV was obtained.

However, the anisotropy of the normal state transport properties: electron motion in the **c**-direction is incoherent in contrast with the metallic behavior of the in-plane electrons as probed by the different ρ_c and ρ_{ab} resistivities^{18,19}, cannot be understood in the current theoretical framework.

The anomalous out of plane behavior of the cuprates has led to the suggestion that conventional Fermi liquid theory fails in these compounds¹. Both theoretical^{1,20,21} and experimental²² work has remarked the relevance of the properties of the direction perpendicular to the CuO_2 planes.

An alternative explanation of the emergence of incoherent behavior in the out of plane direction has been proposed in terms of the coupling of the interlayer electronic motion to charge excitations of the system²¹. This approach implicitly assumes that electron-electron interactions modify the in-plane electron propagators in a non trivial way.

We will show that, even in the clean limit, many body effects can suppress the coherent contribution to the out of plane electron hopping. The clean limit is defined as that in which the length scale, L , over which electrons remain coherent within the layers diverges.

The simplest formulation of the method replaces the excitations of the system (such as electron-hole pairs) by a bath of harmonic oscillators with the same excitation spectrum. This approach can be justified rigorously in one dimension, and is always an accurate description of the response of the system when the coupling of the quasiparticles to each individual excitation is weak²³.

In the following, we will assume a local interaction between electrons close to the Fermi level, and the charge

fluctuations of the system:

$$\mathcal{H}_{int} = c_i^\dagger c_i \sum_{\vec{k}} V_i(\vec{k}) \hat{\rho}_{\vec{k}} \quad (1)$$

where c_i creates an electron at site i , and $\hat{\rho}_{\vec{k}}$ describes the charge fluctuations of the environment, which are to be described as a set of harmonic modes. The Hamiltonian of the system is approximated as:

$$\begin{aligned} \mathcal{H}_{e-b} &= \mathcal{H}_{elec} + \mathcal{H}_{env} + \mathcal{H}_{int} \\ &= \sum \mathbf{t}_{ij} c_i^\dagger c_j + \sum \omega_k b_k^\dagger b_k + \sum g_{k,i} c_i^\dagger c_i (b_k^\dagger + b_k) \end{aligned} \quad (2)$$

where \mathcal{H}_{elec} describes the individual quasiparticles, \mathcal{H}_{env} stands for the set of harmonic oscillators which describe the environment, and \mathcal{H}_{int} defines the (linear) coupling between the two. The b_k^\dagger are boson creation operators, the \mathbf{t}_{ij} describe the electronic hopping processes, and the information about the interaction between the electron in state i and the system is defined by the function²³ $J_i(\omega) = \sum_k |g_{k,i}|^2 \delta(\omega - \omega_k)$.

Using second order perturbation theory and eq.(1), we can write^{23,24}:

$$J_i(\omega) = \sum_{\vec{k}} V_i^2(\vec{k}) \text{Im} \chi(\vec{k}, \omega) \quad (3)$$

where $\chi(\vec{k}, \omega)$ is the Fourier transform of the density-density response of the system, $\langle \hat{\rho}_{\vec{k}}(t) \hat{\rho}_{-\vec{k}}(0) \rangle$. The interaction in eq.(1) is spin independent. Other, more complicated, couplings can also be taken into account, provided that the appropriate response function is used.

The influence of the electron-boson coupling on the electron propagators can be calculated to all orders if the state i is localized, that is, neglecting the hopping terms in eq.(3). We find:

$$\begin{aligned} \langle c_i^\dagger(t) c_i(t') \rangle &\sim \langle c_i^\dagger(t) c_i(t') \rangle_0 \times \\ &\exp \left\{ - \int d\omega \left[1 - e^{i\omega(t-t')} \right] \frac{J_i(\omega)}{\omega^2} \right\} \end{aligned} \quad (4)$$

where $\langle c_i^\dagger(t) c_i(t') \rangle_0 \sim e^{i\varepsilon_i(t-t')}$ is the Green's function in the absence of the interaction. The method that we use assumes that eq.(4) also holds in a system with extended states. For a standard metallic system, we must insert $\langle c_i^\dagger(t) c_i(t') \rangle_0 \sim 1/(t-t')$ in eq.(4). It can be shown that this approximation is exact at short times, $W \ll (t-t')^{-1} \ll \Lambda$, where W is an energy scale related to the dynamics of the electrons, and Λ is the upper cutoff in the spectrum of the environment.

The time dependence in eq.(4) is determined by $\lim_{\omega \rightarrow 0} \chi(\vec{k}, \omega)$. In a gapless, metallic system, we have $\chi(\vec{k}, \omega) \sim \alpha(\vec{k}) |\omega|$. This behavior, when inserted in eq.(4), leads to:

$$\langle c_i^\dagger(t) c_i(t') \rangle \sim \frac{1}{(t-t')^{(1+\alpha)}} \quad (5)$$

where:

$$\alpha = \int_{|\vec{\mathbf{k}}| \ll L^{-1}} d\vec{\mathbf{k}} V^2(\vec{\mathbf{k}}) \alpha(\vec{\mathbf{k}}) \quad (6)$$

where L is the scale of the region where the tunneling process takes place. The value of L is limited by the length over which the phase of the electronic wavefunctions within the layers is well defined. We assume that, in a translationally invariant system, there is no dependence on the position of the local orbital, i . This result implies that the frequency dependence of the Green's function, in a continuum description, can be written as:

$$\lim_{|\vec{\mathbf{r}} - \vec{\mathbf{r}}'| \rightarrow 0} G(\vec{\mathbf{r}} - \vec{\mathbf{r}}', \omega) \propto |\omega|^\alpha \quad (7)$$

We can now use eq.(5) to analyze the interlayer tunneling by applying Renormalization Group methods. The simplest case where this procedure has been used is for the problem of an electron tunneling between two states, i and j , which has been intensively studied^{25,26}. We integrate out the high energy bosons, with energies $\Lambda - d\Lambda \leq \omega_k \leq \Lambda$ and rescaled hopping terms are defined. As mentioned earlier, eq.(5) is valid for this range of energies. The renormalization of the hoppings is such that the properties of the effective Hamiltonian at energies $\omega \ll \Lambda$ remain invariant. If the hoppings \mathbf{t}_{ij} are small, any physical quantity which depends on them can be expanded, using time dependent perturbation theory, in powers of:

$$\mathbf{t}_{ij}^2 \langle c_i^\dagger(t) c_j(t) c_j^\dagger(t') c_i(t') \rangle \approx \mathbf{t}_{ij}^2 \langle c_i^\dagger(t) c_i(t') \rangle \langle c_j(t) c_j^\dagger(t') \rangle \quad (8)$$

The integration of the high energy modes implies that the terms in eq.(8) are restricted to $t \leq \Lambda^{-1}$, or, alternatively, the time unit have to be rescaled²⁷, $\tau' = \tau e^{d\Lambda/\Lambda}$, where $\tau \sim \Lambda^{-1}$. Using eq.(5), the condition of keeping the perturbation expansion in powers of the terms in eq.(8) invariant implies that:

$$\mathbf{t}_{ij}^2 \rightarrow \mathbf{t}_{ij}^2 e^{\frac{d\Lambda}{\Lambda}(2+2\alpha)} \quad (9)$$

which can also be used to define the scaling dimension of the hopping terms. Finally,

$$\frac{\partial(\mathbf{t}_{ij}/\Lambda)}{\partial l} = -\alpha \frac{\mathbf{t}_{ij}}{\Lambda} \quad (10)$$

where $l = \log(\Lambda_0/\Lambda)$, and Λ_0 is the initial value of the cutoff.

This approach has been successfully used to describe inelastic tunneling in different situations in^{21,24,28,29,30,31,32}.

The analysis which leads to eq.(10) can be generalized to study hopping between extended states, provided that we can estimate the long time behavior of the Green's function, $G(\vec{\mathbf{k}}, t - t') = \langle c_{\vec{\mathbf{k}}}^\dagger(t) c_{\vec{\mathbf{k}}}(t') \rangle$. This function is related to the local Green's function, which is written in eq.(7), by:

$$\lim_{|\vec{\mathbf{r}} - \vec{\mathbf{r}}'| \rightarrow 0} G(\vec{\mathbf{r}} - \vec{\mathbf{r}}', \omega) = \int d^D \vec{\mathbf{k}} G(\vec{\mathbf{k}}, \omega) \quad (11)$$

where D is the spatial dimension. In the cases discussed below, the interaction is instantaneous in time, and the non interacting Green's function can be written as:

$$G_0(\vec{\mathbf{k}}, \omega) \propto \frac{1}{\omega} \mathcal{F}\left(\frac{k_i^z}{\omega}\right) \quad (12)$$

where $z = 1, 2$. In the following, we assume that the interacting Green's function has the same scaling properties, with the factor ω^{-1} replaced by $\omega^{-\delta}$ in eq.(12), where δ depends on the interactions. This can be shown to be correct in perturbation theory to all orders, in the models studied below, because the corrections depend logarithmically on ω (it is a well known fact for the Luttinger liquid). Then, using eqs. (7), (11) and (12), we obtain:

$$G(\vec{\mathbf{k}}, \omega) \propto |\omega|^{\alpha-D/z} \mathcal{F}\left(\frac{k_i^z}{\omega}\right) \quad (13)$$

and $\mathcal{F}(u)$ is finite. Thus, from the knowledge of the real space Green's function, using eq.(4), we obtain α , which, in turn, determines the exponent $\alpha + D/z$ which characterizes $G(\vec{\mathbf{k}}, \omega)$. Generically, we can write:

$$G_{l,e}(\omega) \sim |\omega|^{\delta_{l,e}} \quad (14)$$

where the subindices l, e stand for localized and extended wavefunctions. In terms of these exponents, we can generalize eq.(10) to tunneling between general states to:

$$\frac{\partial(\mathbf{t}_{ij}^{l,e}/\Lambda)}{\partial l} = -\delta_{l,e} \frac{\mathbf{t}_{ij}}{\Lambda} \quad (15)$$

Before proceeding to calculations of δ_l and δ_e for various models, it is interesting to note that, in general, the response function of an electron gas in dimension $D > 1$ behaves as $\lim_{\omega \rightarrow 0, |\vec{\mathbf{k}}| \rightarrow 0} \chi(\vec{\mathbf{k}}, \omega) \sim |\omega|/|\vec{\mathbf{k}}|$, so that, from eq.(6), $\lim_{L \rightarrow \infty} \alpha \sim L^{(1-D)}$. Thus, for $D > 1$, the contribution of the inelastic processes to the renormalization of the tunneling vanishes for delocalized states, $L \rightarrow \infty$.

A. Van Hove singularities in the density of states.

The dispersion relation of two-dimensional electronic systems with a square lattice, i.e. the CuO_2 planes of the high- T_c superconductors, usually present Van Hove singularities. The Fermi surface of most hole-doped cuprates is close to a Van Hove singularity. The possible relevance of this fact to the superconducting transition as well as to the anomalous behavior of the normal state was put forward in the early times of the cuprates and gave rise to the so called Van Hove scenario³³. We will assume that the metallic layers are well described by electrons in a square lattice, and that the Fermi level is close to the $(\pi, 0)(A)$ and $(0, \pi)(B)$ points of the Brillouin Zone (BZ). Close to these points, the dispersion relation can be parametrized as:

$$\varepsilon_{A,B}(\vec{\mathbf{k}}) \approx \frac{k_x^2}{2m_{x,y}} \mp \frac{k_y^2}{2m_{y,x}} \quad (16)$$

where m_x and m_y are parameters which can be estimated from the band structure of the model. In the following, we will consider the renormalization of the interlayer tunneling associated to these regions in the BZ.

The response function at low energies and small wavevectors has been computed in³⁴:

$$\text{Im}\chi(\vec{k}, \omega) = \sum_{i=A,B} \frac{1}{4\pi\varepsilon_i(\vec{k})} \left(|\omega + \varepsilon_i(\vec{k})| - |\omega - \varepsilon_i(\vec{k})| \right), \quad (17)$$

where $\varepsilon_i(\vec{k})$ is the dispersion relation (16).

The long time dependence of the Green's function is determined by the low energy behavior of χ : $\lim_{\omega \rightarrow 0} \text{Im} \chi(\vec{k}, \omega) \sim \sum_{i=A,B} |\omega|/\varepsilon_i(\vec{k})$. We assume that the interaction between the electrons and the density fluctuations is short ranged as before. The divergence of $\text{Im}\chi$ when $\varepsilon_{A,B} = 0$ implies that the integral in eq.(6) diverges logarithmically as $L \rightarrow \infty$, as in the two previous cases, irrespective of the details of the interaction, $V(\vec{k})$. Because of this divergence, it is convenient to shift slightly the chemical potential ε_F away from the saddle point³⁴, ε_{VH} . A finite value of $|\varepsilon_F - \varepsilon_{VH}|$ implies the existence of a length scale, $L_0 \sim [\text{Max}(m_x, m_y)|\varepsilon_F - \varepsilon_{VH}|]^{-1/2}$, which regularizes the \vec{k} integrals in eq.(6).

Using a local potential, we find:

$$\alpha \sim (U/W)^2 \log^2(L/L_0) \quad (18)$$

where W is an energy scale of the order of the width of the conduction band. The dependence of α on L goes as $\log^2(L)$, as in other physical quantities in this model³⁴.

In the two dimensional model, $z = 2$, so that $\delta_l = \alpha$, as estimated above, and $\delta_e = \alpha - 1$. The divergence of α implies that tunneling between localized and also between extended states is suppressed at low temperatures. In addition, the effective electron-electron coupling, U , grows at low energies or temperatures, until a scale at which the system is unstable and a phase transition takes place³⁴. This effect enhances the suppression of interlayer hopping.

III. BILAYER BAND SPLITTING

To study de bilayer band splitting (BS) we apply the method described above and consider the interlayer tunnelling between two CuO_2 planes within the Van Hove scenario. We will consider the electronic states near the two inequivalent saddle points of the square lattice. The lowest order corrections to the bare couplings included in the $t-t'$ - Hubbard Hamiltonian, will give the anisotropic screening of the interactions³⁴, by the Kohn-Luttinger mechanism, in contrast to the isotropic three-dimensional metal³⁵. The parameters of the model will be the interlayer hopping, the distance of the Fermi level ε_F to the Van Hove singularity ε_{VH} given by the band structure, the band width W and the strength of the interaction α .

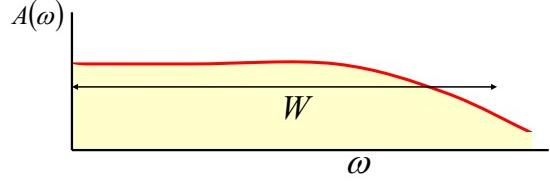


FIG. 1: Schematic representation of spectral function $A(\omega)$ versus frequency for the strong coupling case. The band width W indicates the high-energy cutoff.

The effective Hamiltonian will be defined at each scale of the couplings. The $|\varepsilon_{VH} - \varepsilon_F|$ defines the low energy cutoff while the bandwidth W defines the high-energy cutoff of the Renormalization Group approach. The hopping renormalization gives the $t_{eff} \approx t \left(\frac{|\varepsilon_{VH} - \varepsilon_F|}{W} \right)^\alpha$

We analyze the phase diagram relating the strength of the couplings to the doping level. The underdoped regime would correspond to the strongly correlated system. The interaction $\alpha > 1$, the Van Hove singularity lies at the Fermi level so that the low-energy cutoff $|\varepsilon_{VH} - \varepsilon_F| = 0$; no BS occurs at this regime, a broad structureless background will extend in the scale of W as it is shown in Fig 1.

The system is instable at low energies, and low temperature phase transition to the superconducting phase are highly probable. The underdoped-optimally doped regime would correspond as well to strongly correlated system, $\alpha > 1$, but in the frequency region below the low-energy cutoff a renormalized bilayer splitting will appear, since quasiparticles would be renormalized. The renormalization factor depends on the cutoffs as

$$Z = \left(\frac{|\varepsilon_{VH} - \varepsilon_F|}{W} \right)^\alpha$$

Between the low and high energy cutoffs, a broad background without any structure would be obtained, as schematically represented in Figure 2.

The overdoped regime, as stated above, would correspond to the weakly correlated case, $\alpha < 1$. Electron correlations are screened and, as schematically represented in Figure 3, the renormalization of the bilayer splitting would be weaker than in the preceding case. An incoherent tail of the spectral weight is shown with a power law decay at high energies, $A(\omega) \approx \frac{C}{\omega^{1-\alpha}} \sin(\pi\alpha/2)$ always below the high-energy cutoff.

IV. CONCLUSIONS.

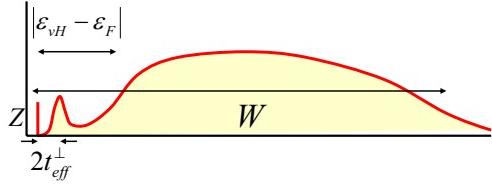


FIG. 2: Same as Fig.1 with renormalized bilayer splitting at frequencies below the low-energy cutoff, $|\epsilon_{VH} - \epsilon_F|$. The band width W indicates the high-energy cutoff.

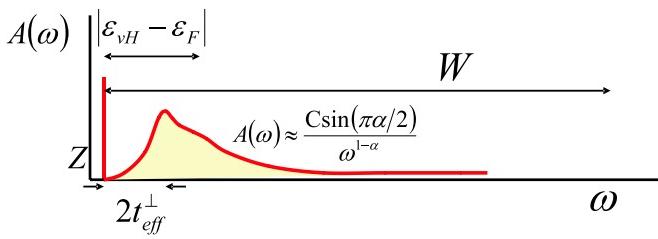


FIG. 3: Same as Fig.1 with bilayer splitting at frequencies below the low-energy cutoff, $|\epsilon_{VH} - \epsilon_F|$. The spectral weight decays at high energies. The band width W indicates the high-energy cutoff.

The effects of electron-electron correlations on the out-of-plane properties of layered systems have been studied. We have discussed the suppression of interlayer tunneling by inelastic processes in two dimensional systems in the clean limit. Our results suggest that, when perturbation theory for the in-plane interactions leads to logarithmic divergences, the out of plane tunneling acquires a non trivial energy dependence. The conductance goes to zero as $T \rightarrow 0$ if the Fermi level of the interacting electrons lies at a Van Hove singularity. Coherence would be suppressed and the bilayer splitting would vanish as a consequence of the strong correlations. When $|\epsilon_{VH} - \epsilon_F| \neq 0$, a strongly renormalized bilayer splitting occurs below $|\epsilon_{VH} - \epsilon_F|$ which marks the low-energy cutoff of the system. These two situations correspond to the underdoped and optimally doped regions in the cuprate scenario. In the overdoped case, quasiparticles would be weakly renormalized and the bilayer splitting will be present.

Thus, we have shown that insulating behavior in the out of plane direction is not incompatible with gapless or even superconducting in-plane properties, although the in plane properties are also markedly different from those of an ordinary Fermi liquid.

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